

# The rotationally invariant approximation for the two-dimensional $t$ - $J$ model

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(February 1, 2008)

## Abstract

Using the description in terms of the Hubbard operators hole and spin Green's functions of the two-dimensional  $t$ - $J$  model are calculated in an approximation which retains the rotation symmetry of the spin susceptibility in the paramagnetic state and has no predefined magnetic ordering. In this approximation, Green's functions are represented by continued fractions which are interrupted with the help of the decoupling corrected by the constraint of zero site magnetization in the paramagnetic state. Results obtained in this approach for an undoped  $32 \times 32$  lattice (the Heisenberg model) and for one hole in a  $4 \times 4$  lattice are in good agreement with Monte Carlo and exact diagonalization data, respectively. In the limit of heavy doping the hole spectrum described by the obtained formulas acquires features of the spectrum of weakly correlated excitations.

PACS numbers: 71.10.Fd, 71.27.+a, 74.25.Ha, 74.25.Jb

## I. INTRODUCTION

The two-dimensional  $t$ - $J$  model is one of the most frequently used models for the description of  $\text{CuO}_2$  planes of perovskite high- $T_c$  superconductors (for a review, see Ref. 1). Together with the numerical methods – the exact diagonalization of small clusters,<sup>2,3</sup> Monte Carlo simulations<sup>4</sup> and the density-matrix renormalization-group technique<sup>5</sup> – a number of analytical methods, such as the mean-field slave-boson<sup>6</sup> and spin-wave approximations, was used for the investigation of the model. The latter method which is based on the spin-wave description of the magnetic excitations was shown to be remarkably accurate in the case of small hole concentrations and zero temperature.<sup>7</sup> This approach was extended to the ranges of moderate hole concentrations and finite temperatures,<sup>8</sup> in particular with the use of the spin-wave approximation modified<sup>9</sup> for short-range order.<sup>10</sup> The positions, symmetry and size of the pseudogaps in the hole and magnon spectra, values of the magnetic susceptibility and spin-lattice relaxation rates obtained in this approach are close to those observed in photoemission, spin-lattice relaxation and neutron scattering experiments on cuprate perovskites.<sup>10,11</sup>

The apparent shortcomings of the spin-wave approximation of the  $t$ - $J$  model are the violation of the rotation symmetry of the spin susceptibility components in the paramagnetic state, the predefined magnetic ordering in the Néel state which serves as the reference state of the approximation, and the neglect of the kinematic interaction. In this paper we try to overcome these shortcomings by using the description in terms of Hubbard operators. Green's functions constructed from these operators are calculated with the use of the continued fraction representations following from the Mori projection procedure.<sup>12</sup> To interrupt these otherwise infinite continued fractions we use decouplings of the higher-order Green's functions arising in later stages of this calculation procedure. Following the idea of Ref. 13, a correction parameter is introduced in these decouplings to fulfill the constraint of zero site magnetization in the paramagnetic state. In this state the obtained components of the spin Green's functions are rotationally invariant. The self-energy equations are similar in their form to the equations derived in the modified spin-wave approximation.<sup>10</sup> In the case of heavy doping the pole in the hole Green's function corresponds to a weakly correlated nearest-neighbor band. To check the validity of the obtained equations in the opposite case of light doping we have performed calculations for conditions which allow comparison with exact diagonalization and Monte Carlo results. We found good agreement of our results with the results of Refs. 2,14 for spin correlations in an undoped  $32 \times 32$  lattice and for the hole spectral function of a  $4 \times 4$  lattice with one hole. To gain a notion of the spectral function in larger lattices it was calculated in a  $20 \times 20$  cluster.

## II. DESCRIPTION OF THE MODEL

The Hamiltonian of the two-dimensional  $t$ - $J$  model reads

$$H = \sum_{\mathbf{n}\mathbf{m}\sigma} t_{\mathbf{n}\mathbf{m}} a_{\mathbf{n}\sigma}^\dagger a_{\mathbf{m}\sigma} + \frac{1}{2} \sum_{\mathbf{n}\mathbf{m}} J_{\mathbf{n}\mathbf{m}} (s_{\mathbf{n}}^z s_{\mathbf{m}}^z + s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1}) + \mu \sum_{\mathbf{n}} X_{\mathbf{n}}, \quad (1)$$

where  $a_{\mathbf{n}\sigma} = |\mathbf{n}\sigma\rangle\langle\mathbf{n}0|$  is the hole annihilation operator,  $\mathbf{n}$  and  $\mathbf{m}$  label sites of the square lattice,  $\sigma = \pm 1$  is the spin projection,  $|\mathbf{n}\sigma\rangle$  and  $|\mathbf{n}0\rangle$  are site states corresponding to the

absence and presence of a hole on the site. If Hamiltonian (1) is obtained from the extended Hubbard Hamiltonian,<sup>15</sup> these states are linear combinations of the products of the respective  $3d_{x^2-y^2}$  copper and  $2p_\sigma$  oxygen orbitals.<sup>10</sup> We take into account nearest neighbor interactions only,  $t_{\mathbf{n}\mathbf{m}} = t \sum_{\mathbf{a}} \delta_{\mathbf{n},\mathbf{m}+\mathbf{a}}$  and  $J_{\mathbf{n}\mathbf{m}} = J \sum_{\mathbf{a}} \delta_{\mathbf{n},\mathbf{m}+\mathbf{a}}$  where  $t$  and  $J$  are hopping and exchange constants and the four vectors  $\mathbf{a}$  connect nearest neighbor sites. The spin- $\frac{1}{2}$  operators can be written in the Dirac notations as  $s_{\mathbf{n}}^z = \frac{1}{2} \sum_{\sigma} \sigma |\mathbf{n}\sigma\rangle\langle\mathbf{n}\sigma|$  and  $s_{\mathbf{n}}^\sigma = |\mathbf{n}\sigma\rangle\langle\mathbf{n}, -\sigma|$ . The chemical potential  $\mu$  is included into Hamiltonian (1) to control the hole concentration.  $X_{\mathbf{n}} = |\mathbf{n}0\rangle\langle\mathbf{n}0|$ . The term  $-\frac{J}{8} \sum_{\mathbf{n}\mathbf{a}} X_{\mathbf{n}} X_{\mathbf{n}+\mathbf{a}}$  is frequently included into Hamiltonian (1). For problems considered below this term leads to an unessential renormalization of the chemical potential and therefore it is omitted. The operators  $a_{\mathbf{n}\sigma}$ ,  $s_{\mathbf{n}}^z$ ,  $s_{\mathbf{n}}^\sigma$ , and  $X_{\mathbf{n}}$  are the Hubbard operators in the space of states of the  $t$ - $J$  model.

The states  $|\mathbf{n}\sigma\rangle$  and  $|\mathbf{n}0\rangle$  satisfy the following completeness condition:

$$\sum_{\sigma} |\mathbf{n}\sigma\rangle\langle\mathbf{n}\sigma| + |\mathbf{n}0\rangle\langle\mathbf{n}0| = 1. \quad (2)$$

Using this condition and the above expression for  $s_{\mathbf{n}}^z$  the constraint of zero site magnetization, which has to be fulfilled in the paramagnetic state, can be reduced to the form

$$\langle s_{\mathbf{n}}^z \rangle = \frac{1}{2} (1 - x) - \langle s_{\mathbf{n}}^{-1} s_{\mathbf{n}}^{+1} \rangle = 0, \quad (3)$$

where angular brackets denote averaging over the grand canonical ensemble and the hole concentration  $x = \langle X_{\mathbf{n}} \rangle$  in the homogeneous state. It should be noticed that in accord with the Mermin-Wagner theorem<sup>16</sup> the long-range antiferromagnetic ordering is destroyed for any nonzero temperature in the two-dimensional system. Therefore the fulfillment of constraint (3) has to be ensured for the considered states.

The above operators satisfy the following commutation (anticommutation) relations:

$$\begin{aligned} [s_{\mathbf{n}}^{-1}, s_{\mathbf{m}}^{+1}] &= -2s_{\mathbf{n}}^z \delta_{\mathbf{n}\mathbf{m}}, & [s_{\mathbf{n}}^\sigma, s_{\mathbf{m}}^z] &= -\sigma s_{\mathbf{n}}^\sigma \delta_{\mathbf{n}\mathbf{m}}, \\ [a_{\mathbf{n}\sigma}, s_{\mathbf{m}}^z] &= -\frac{1}{2} \sigma a_{\mathbf{n}\sigma} \delta_{\mathbf{n}\mathbf{m}}, & [a_{\mathbf{n}\sigma}, s_{\mathbf{m}}^{\sigma'}] &= -a_{\mathbf{n},-\sigma} \delta_{\mathbf{n}\mathbf{m}} \delta_{\sigma,-\sigma'}, \\ \{a_{\mathbf{n}\sigma}, a_{\mathbf{m},\sigma'}^\dagger\} &= (1 - s_{\mathbf{n}}^{-\sigma} s_{\mathbf{n}}^\sigma) \delta_{\mathbf{n}\mathbf{m}} \delta_{\sigma\sigma'} + s_{\mathbf{n}}^\sigma \delta_{\mathbf{n}\mathbf{m}} \delta_{\sigma,-\sigma'}, & \{a_{\mathbf{n}\sigma}, a_{\mathbf{m}\sigma'}\} &= 0, \\ [s_{\mathbf{n}}^{-1}, X_{\mathbf{m}}] &= 0, & [s_{\mathbf{n}}^z, X_{\mathbf{m}}] &= 0, & [a_{\mathbf{n}\sigma}, X_{\mathbf{m}}] &= a_{\mathbf{n}\sigma} \delta_{\mathbf{n}\mathbf{m}}. \end{aligned} \quad (4)$$

Notice that the hole creation and annihilation operators do not satisfy the fermion anticommutation relations. This is the consequence of the exclusion of doubly occupied site states due to the strong on-site repulsion [see Eq. (2)].

### III. CONTINUED FRACTION REPRESENTATION OF GREEN'S FUNCTIONS

To investigate the energy spectrum and magnetic properties we shall calculate the hole and spin retarded Green's functions

$$G(\mathbf{k}t) = \langle\langle a_{\mathbf{k}\sigma} | a_{\mathbf{k}\sigma}^\dagger \rangle\rangle_t = -i\theta(t) \langle\{a_{\mathbf{k}\sigma}(t), a_{\mathbf{k}\sigma}^\dagger\}\rangle, \quad D(\mathbf{k}t) = \langle\langle s_{\mathbf{k}}^z | s_{-\mathbf{k}}^z \rangle\rangle_t = -i\theta(t) \langle[s_{\mathbf{k}}^z(t), s_{-\mathbf{k}}^z]\rangle, \quad (5)$$

where  $a_{\mathbf{k}\sigma} = N^{-1/2} \sum_{\mathbf{n}} \exp(-i\mathbf{k}\mathbf{n}) a_{\mathbf{n}\sigma}$ ,  $s_{\mathbf{k}}^z = N^{-1/2} \sum_{\mathbf{n}} \exp(-i\mathbf{k}\mathbf{n}) s_{\mathbf{n}}^z$ ,  $N$  is the number of sites and  $a_{\mathbf{k}\sigma}(t) = \exp(iHt) a_{\mathbf{k}\sigma} \exp(-iHt)$ . In the considered states  $G(\mathbf{k}t)$  does not depend on  $\sigma$ .

To calculate the above Green's functions we use their continued fraction representations which can be obtained using the Mori projection operator technique.<sup>12</sup> Let us consider the inner product  $|A \cdot B^\dagger|$  of the operators  $A$  and  $B$  which is defined in such a manner that the following conditions are fulfilled: i)  $|(aA + bB) \cdot C^\dagger| = a|A \cdot C^\dagger| + b|B \cdot C^\dagger|$ ,  $a$  and  $b$  are arbitrary numbers; ii)  $|[A, H] \cdot B^\dagger| = |A \cdot [H, B^\dagger]|$ ; iii)  $|A \cdot B^\dagger| = |B \cdot A^\dagger|^*$ . We notice that the inner products defined as  $\langle \{A, B^\dagger\} \rangle$ ,  $\langle [A, B^\dagger] \rangle$ , and

$$(A, B^\dagger) = i \int_0^\infty dt e^{-\eta t} \langle [A(t), B^\dagger] \rangle, \quad \eta \rightarrow +0 \quad (6)$$

satisfy the above properties. Let us divide the result of the commutation of some operator  $A_0$  with the Hamiltonian into longitudinal and transversal parts with respect to  $A_0$ . The transversal part  $A_1$  is determined as an operator the inner product of which with  $A_0$  is equal to zero. Thus,

$$[A_0, H] = E_0 A_0 + A_1, \quad (7)$$

where  $E_0$  is determined from the condition  $|A_1 \cdot A_0^\dagger| = 0$ ,

$$E_0 = |[A_0, H] \cdot A_0^\dagger| |A_0 \cdot A_0^\dagger|^{-1}.$$

Given  $A_0$  and  $E_0$ , the operator  $A_1$  may be found from Eq. (7). The commutator of  $A_1$  with the Hamiltonian will contain already three terms,

$$[A_1, H] = E_1 A_1 + A_2 + F_0 A_0.$$

The coefficients  $E_1$  and  $F_0$  and the new operator  $A_2$  are determined with the use of the two orthogonality conditions  $|A_2 \cdot A_i^\dagger| = 0$ ,  $i = 0, 1$ ,

$$E_1 = |[A_1, H] \cdot A_1^\dagger| |A_1 \cdot A_1^\dagger|^{-1}, \quad F_0 = |[A_1, H] \cdot A_0^\dagger| |A_0 \cdot A_0^\dagger|^{-1} = |A_1 \cdot A_1^\dagger| |A_0 \cdot A_0^\dagger|^{-1},$$

where we have used the properties of the inner product. This procedure can be continued. In each step of it the coefficients and a new operator are determined by the conditions of the orthogonality of this operator to all operators obtained previously. Using the properties of the inner product it can be shown that only the  $n$ -th,  $(n+1)$ -th and  $(n-1)$ -th operators appear in the commutator of the  $n$ -th operator with the Hamiltonian,<sup>17</sup>

$$[A_n, H] = E_n A_n + A_{n+1} + F_{n-1} A_{n-1}, \quad (8)$$

$$E_n = |[A_n, H] \cdot A_n^\dagger| |A_n \cdot A_n^\dagger|^{-1}, \quad F_{n-1} = |A_n \cdot A_n^\dagger| |A_{n-1} \cdot A_{n-1}^\dagger|^{-1}.$$

As can be seen, algorithm (8) is the modification of the Lanczos orthogonalization procedure which is well known in computational mathematics (see, e.g., Ref. 18 and references therein)

and physics.<sup>19</sup> In Eq. (8), operators  $A_n$  play the role of mutually orthogonal wave functions or vectors in the usual Lanczos procedure.

Following Mori<sup>12</sup> we introduce the projection operator  $P_n$  which projects an arbitrary operator  $Q$  on the operator  $A_n$ ,

$$P_n Q = |Q \cdot A_n^\dagger| |A_n \cdot A_n^\dagger|^{-1} A_n,$$

and determine the time evolution of the operator  $A_n$  by the equation

$$i \frac{d}{dt} A_{nt} = \prod_{k=0}^{n-1} (1 - P_k) [A_{nt}, H], \quad A_{n,t=0} = A_n, \quad (9)$$

Due to the projection operators in Eq. (9) this time dependence of the operator differs from the conventional one except the dependence of  $A_0$ . To underline this difference we use the subscript notation for the time dependence in Eq. (9). Notice also that in accord with this equation  $A_{nt}$  remains orthogonal to operators  $A_i$ ,  $i < n$  for  $t > 0$ . Let us divide  $A_{nt}$  into two parts,

$$A_{nt} = R_n(t) A_n + A'_{nt}, \quad R_n(t) = |A_{nt} \cdot A_n^\dagger| |A_n \cdot A_n^\dagger|^{-1}.$$

From this definition it follows that  $A'_{nt} = (1 - P_n) A_{nt}$ . Equations (8) and (9) determine the time evolution of this operator,

$$i \frac{d}{dt} A'_{nt} = R_n(t) A_{n+1} + \prod_{k=0}^n (1 - P_k) [A'_{nt}, H].$$

Solving this equation we find

$$A_{nt} = R_n(t) A_n - i \int_0^t d\tau R_n(\tau) A_{n+1,t-\tau}.$$

This result allows us to obtain the following equation for the functions  $R_n(t)$ :

$$i \frac{d}{dt} R_n(t) = E_n R_n(t) - i F_n \int_0^t d\tau R_n(\tau) R_{n+1}(t - \tau).$$

After the Laplace transformation  $R_n(\omega) = -i \int_0^\infty dt \exp(i\omega t) R_n(t)$  this equation reads

$$R_n(\omega) = [\omega - E_n - F_n R_{n+1}(\omega)]^{-1}. \quad (10)$$

If the inner product is defined as the average of the commutator (anticommutator) of operators, the function  $\tilde{R}_0(\omega) = R_0(\omega) |A_0 \cdot A_0^\dagger|$  coincides with the Fourier transform,  $\langle\langle A_0 | A_0^\dagger \rangle\rangle_\omega = \int_{-\infty}^\infty dt \exp(i\omega t) \langle\langle A_0 | A_0^\dagger \rangle\rangle_t$ , of the commutator (anticommutator) retarded Green's functions of the type of Eq. (5). If the inner product is defined by Eq. (6), the function  $\tilde{R}_0(\omega)$  coincides with Kubo's relaxation function

$$\left( (A_0 | A_0^\dagger) \right)_\omega = \int_{-\infty}^\infty dt e^{i\omega t} \left( (A_0 | A_0^\dagger) \right)_t, \quad \left( (A_0 | A_0^\dagger) \right)_t = \theta(t) \int_t^\infty dt' \langle [A_0(t'), A_0^\dagger] \rangle. \quad (11)$$

From Eq. (10) for all these functions we obtain the following continued fraction representation:

$$\tilde{R}_0(\omega) = \frac{|A_0 \cdot A_0^\dagger|}{\omega - E_0 - \frac{F_0}{\omega - E_1 - \frac{F_1}{\ddots}}}. \quad (12)$$

Thus the recursive procedure (8) in course of which the coefficients  $E_n$  and  $F_n$  of the continued fraction (12) are determined allows us to calculate Green's or Kubo's relaxation functions.

#### IV. THE SPIN GREEN'S FUNCTION

The direct application of Eqs. (8) and (12) to the spin Green's function  $D(\mathbf{k}\omega)$ , Eq. (5), meets with difficulties because the inner product  $\langle [s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z] \rangle$  in the numerator of the continued fraction (12) is equal to zero. To overcome this difficulty we consider Kubo's relaxation function  $((s_{\mathbf{k}}^z | s_{-\mathbf{k}}^z))$  defined in Eq. (11). In this case the inner product (6) in the numerator of the respective continued fraction is nonzero. After calculating the relaxation function the spin Green's function can be obtained from the relation

$$\omega ((s_{\mathbf{k}}^z | s_{-\mathbf{k}}^z)) = \langle \langle s_{\mathbf{k}}^z | s_{-\mathbf{k}}^z \rangle \rangle + (s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z), \quad (13)$$

where we dropped the subscript  $\omega$  in the relaxation and Green's functions.

We postpone the calculation of the numerator  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$  of the continued fraction and consider its other coefficients. From definition (6) we find that  $E_0(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z) = (i\dot{s}_{\mathbf{k}}^z, s_{-\mathbf{k}}^z) = \langle [s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z] \rangle = 0$  and therefore  $A_1$  is the Fourier transform of the operator

$$i\dot{s}_1^z = \frac{1}{2} \sum_{\mathbf{mn}} J_{\mathbf{mn}} (\delta_{\mathbf{ln}} - \delta_{\mathbf{lm}}) s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1} + \frac{1}{2} \sum_{\mathbf{mn}\sigma} t_{\mathbf{mn}} \sigma (\delta_{\mathbf{lm}} - \delta_{\mathbf{ln}}) a_{\mathbf{n}\sigma}^\dagger a_{\mathbf{m}\sigma} = \mathcal{A}_1^s + \mathcal{A}_1^h. \quad (14)$$

Here the dot over the operator indicates the time derivative. As can be seen,  $A_1$  contains contributions from spin and hole components  $\mathcal{A}^s$  and  $\mathcal{A}^h$ . Using this result in calculating  $R_1(\omega)$  which is the Laplace transform of the function  $(A_{1t}, A_1^\dagger)$  we neglect the terms  $(\mathcal{A}_{1t}^h, \mathcal{A}^{s\dagger})$  and  $(\mathcal{A}_{1t}^s, \mathcal{A}^{h\dagger})$ . This approximation is motivated by vanishing values of these correlations obtained with the decoupling. Therefore

$$(A_{1t}, A_1^\dagger) \approx (\mathcal{A}^h(t), \mathcal{A}^{h\dagger}) + (\mathcal{A}_{1t}^s, \mathcal{A}^{s\dagger}), \quad (15)$$

where we have additionally neglected the difference between  $\mathcal{A}_{1t}^h$  and  $\mathcal{A}^h(t)$  (again due to zero values of the respective decoupling). In accord with our estimation the influence of terms connected with holes in  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$  and  $((\mathcal{A}_{\mathbf{k}}^s | \mathcal{A}_{\mathbf{k}}^{s\dagger}))$  on the spin Green's function is small in comparison with the quantity  $((\mathcal{A}_{\mathbf{k}}^h | \mathcal{A}_{\mathbf{k}}^{h\dagger}))$  even for moderate hole concentrations. Therefore in the forthcoming discussion we neglect these terms in  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$  and  $((\mathcal{A}_{\mathbf{k}}^s | \mathcal{A}_{\mathbf{k}}^{s\dagger}))$  and consider the time evolution of operators in these quantities as determined solely by the Heisenberg part of Hamiltonian (1). In this approximation the numerator of the continued fraction representing  $((\mathcal{A}_{\mathbf{k}}^s | \mathcal{A}_{\mathbf{k}}^{s\dagger}))$  reads

$$(\mathcal{A}_{\mathbf{k}}^s, \mathcal{A}_{\mathbf{k}}^{s\dagger}) = (i\dot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z) = \langle [i\dot{s}_{\mathbf{k}}^z, s_{-\mathbf{k}}^z] \rangle = 4JC_1(\gamma_{\mathbf{k}} - 1), \quad (16)$$

where  $\gamma_{\mathbf{k}} = \frac{1}{4} \sum_{\mathbf{a}} \exp(i\mathbf{k}\mathbf{a})$ ,  $C_p = \frac{1}{N} \sum_{\mathbf{k}} \gamma_{\mathbf{k}}^p C_{\mathbf{k}}$  and  $C_{\mathbf{k}} = \sum_{\mathbf{n}} \exp[i\mathbf{k}(\mathbf{n} - \mathbf{m})] \langle s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1} \rangle$ . For  $E_1$  we get  $E_1(i\dot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z) = (i^2\ddot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z) = \langle [i\dot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z] \rangle = 0$ . Thus, breaking off the continued fraction on this step we obtain from Eqs. (12), (13), (15) and (16)

$$D(\mathbf{k}\omega) = \frac{\omega \left( (\mathcal{A}_{\mathbf{k}}^h | \mathcal{A}_{\mathbf{k}}^{h\dagger}) \right) + 4JC_1(\gamma_{\mathbf{k}} - 1)}{\omega^2 - 2\omega \Pi(\mathbf{k}\omega) - \omega_{\mathbf{k}}^2}, \quad (17)$$

where the polarization operator and the excitation frequency are given by

$$\Pi(\mathbf{k}\omega) = \frac{1}{2} \left( (\mathcal{A}_{\mathbf{k}}^h | \mathcal{A}_{\mathbf{k}}^{h\dagger}) \right) (s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)^{-1}, \quad \omega_{\mathbf{k}}^2 = 4JC_1(\gamma_{\mathbf{k}} - 1) (s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)^{-1}. \quad (18)$$

To calculate  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$  in the above formulas we notice that in the considered case  $A_2 = i^2\ddot{s}_{\mathbf{k}}^z - (i\dot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z) (s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)^{-1} s_{\mathbf{k}}^z$  and

$$(A_2, A_2^\dagger) = \langle [i^2\ddot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z] \rangle - \frac{16J^2C_1^2(\gamma_{\mathbf{k}} - 1)^2}{(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)} = 0. \quad (19)$$

We set the above result equal to zero in conformity with the approximation made above in the continued fraction where we dropped all terms containing  $A_2$  and operators of higher orders. Equation (19) can be used for calculating  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$  if the value of  $\langle [i^2\ddot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z] \rangle$  is known. An analogous equation was obtained in Ref. 20 with another method.

We calculate  $\langle [i^2\ddot{s}_{\mathbf{k}}^z, -i\dot{s}_{-\mathbf{k}}^z] \rangle$  in Eq. (19) by decoupling terms in the second derivative of  $s^z$ ,

$$i\ddot{s}_{\mathbf{l}}^z = \frac{1}{2} \sum_{\mathbf{mn}} \left[ J_{\mathbf{lm}} J_{\mathbf{ln}} (2s_{\mathbf{l}}^z s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1} - s_{\mathbf{n}}^z s_{\mathbf{l}}^{+1} s_{\mathbf{m}}^{-1} - s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^z s_{\mathbf{l}}^{-1}) + \right. \\ \left. J_{\mathbf{lm}} J_{\mathbf{mn}} (s_{\mathbf{n}}^z s_{\mathbf{m}}^{+1} s_{\mathbf{l}}^{-1} - s_{\mathbf{m}}^z s_{\mathbf{n}}^{+1} s_{\mathbf{l}}^{-1} + s_{\mathbf{l}}^{+1} s_{\mathbf{n}}^z s_{\mathbf{m}}^{-1} - s_{\mathbf{l}}^{+1} s_{\mathbf{m}}^z s_{\mathbf{n}}^{-1}) \right]. \quad (20)$$

In the decoupling we approximate  $s_{\mathbf{l}}^z s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1}$  by the value  $[\alpha C_{\mathbf{nm}} (1 - \delta_{\mathbf{nm}}) + \frac{1}{2} \delta_{\mathbf{nm}}] s_{\mathbf{l}}^z$  where  $C_{\mathbf{nm}} = \langle s_{\mathbf{n}}^{+1} s_{\mathbf{m}}^{-1} \rangle$ . In the last expression we took into account that in accordance with Eq. (3)  $C_{\mathbf{nn}} = \frac{1}{2}$  for  $x = 0$  [let us remind that we neglect the influence of holes on the value of  $(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)$ ]. Following Ref. 13 the parameter  $\alpha$  is introduced to fulfill the constraint of zero site magnetization (3) in the paramagnetic state. Before carrying out the decoupling it has to be taken into account that terms of Eq. (20) in which the site index of the  $s^z$  operator coincides with the site index of  $s^{+1}$  or  $s^{-1}$  operators cancel each other. To verify this statement it is necessary to take into consideration that in these terms the operators  $s_{\mathbf{n}}^z$  can be substituted by  $-\frac{1}{2}$ , since for the spin- $\frac{1}{2}$  case  $s_{\mathbf{n}}^z = -\frac{1}{2} + s_{\mathbf{n}}^{+1} s_{\mathbf{n}}^{-1}$  and  $s_{\mathbf{n}}^{+1} s_{\mathbf{n}}^{+1} = 0$ . To retain this exact cancellation it has to be taken into account before the decoupling. As the result we find

$$i^2\ddot{s}_{\mathbf{l}}^z = \alpha \sum_{\mathbf{mn}} \left[ J_{\mathbf{lm}} J_{\mathbf{ln}} (C_{\mathbf{mn}} s_{\mathbf{l}}^z - C_{\mathbf{lm}} s_{\mathbf{n}}^z) + J_{\mathbf{ln}} J_{\mathbf{mn}} (C_{\mathbf{ln}} s_{\mathbf{m}}^z - C_{\mathbf{lm}} s_{\mathbf{n}}^z) \right] \\ + \sum_{\mathbf{n}} J_{\mathbf{ln}}^2 \left[ (1 - \alpha) C_{\mathbf{nn}} (s_{\mathbf{l}}^z - s_{\mathbf{n}}^z) + \alpha C_{\mathbf{ln}} (s_{\mathbf{n}}^z - s_{\mathbf{l}}^z) \right],$$

and after the Fourier transformation

$$i^2 \ddot{s}_{\mathbf{k}}^z = \omega_{\mathbf{k}}^2 s_{\mathbf{k}}^z,$$

where

$$\omega_{\mathbf{k}}^2 = \frac{\langle [i^2 \ddot{s}_{\mathbf{k}}^z, -i \dot{s}_{-\mathbf{k}}^z] \rangle}{4J C_1 (\gamma_{\mathbf{k}} - 1)} = 16J^2 \alpha |C_1| (1 - \gamma_{\mathbf{k}}) (\Delta + 1 + \gamma_{\mathbf{k}}), \quad (21)$$

$$\Delta = \frac{C_2}{|C_1|} + \frac{1 - \alpha}{8\alpha |C_1|} - \frac{3}{4}.$$

Combining Eqs. (16), (18) and (21) we find

$$(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)^{-1} = 4J\alpha (\Delta + 1 + \gamma_{\mathbf{k}}). \quad (22)$$

In the absence of holes Eqs. (17) and (21) are close to the equations for the spin Green's function and the excitation frequency obtained for the two-dimensional Heisenberg antiferromagnet in Ref. 21,22 with the use of the equations of motion for Green's functions and Tserkovnikov's formalism,<sup>20</sup> respectively. In these works, somewhat more complicated decouplings were used. These decouplings contain several decoupling parameters of the type of  $\alpha$  which depend on the site indices in the decoupled average. These additional parameters allow one to obtain somewhat better agreement with numeric simulations. However, to fix the additional parameters exterior data from numerical simulations or the spin-wave theory have to be engaged and the theory ceases to be closed.

As can be shown by the analogous calculation of the transversal spin Green's function  $\langle\langle s_{\mathbf{k}}^{-1} | s_{\mathbf{k}}^{+1} \rangle\rangle$ , in the paramagnetic state

$$\langle\langle s_{\mathbf{k}}^{-1} | s_{\mathbf{k}}^{+1} \rangle\rangle = 2 \langle\langle s_{\mathbf{k}}^z | s_{-\mathbf{k}}^z \rangle\rangle. \quad (23)$$

Thus, the rotation symmetry of the components of the magnetic susceptibility is retained in this approach. This fact can be used for the calculation of parameters  $C_1$ ,  $C_2$  and  $\alpha$  in the above formulas. From Eq. (17) simplified for the absence of holes, Eq. (23) and the relation

$$\langle s_{\mathbf{k}}^z(t) s_{-\mathbf{k}}^z \rangle = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} e^{\beta\omega} n_B(\omega) B(\mathbf{k}\omega), \quad (24)$$

we find

$$C_{\mathbf{k}} = 4J |C_1| (1 - \gamma_{\mathbf{k}}) \omega_{\mathbf{k}}^{-1} \coth \left( \frac{1}{2} \beta \omega_{\mathbf{k}} \right), \quad (25)$$

where  $B(\mathbf{k}E) = -\pi^{-1} \text{Im } D(\mathbf{k}E)$  is the spin spectral function,  $n_B(E) = [\exp(\beta E) - 1]^{-1}$  and  $\beta = T^{-1}$  is the inverse temperature. Substituting this equation in the definitions of  $C_1$ ,  $C_2$  and in constraint (3) we obtain three equations for the three unknown parameters  $C_1$ ,  $C_2$  and  $\alpha$ . This problem can be reduced to the optimization problem and solved by the steepest descent method.

To check the validity of the approximations made above we used the obtained formulas for calculating spin correlations in an undoped antiferromagnet. In Fig. 1 our results obtained



in a  $32 \times 32$  lattice for three temperatures are compared with data of Monte Carlo simulations performed for the same lattice in Ref. 14. As can be seen, the agreement is good. However, it should be noted that at elevated temperatures in our approximation the spin correlations are systematically overestimated in comparison with the Monte Carlo results.

As follows from Eq. (21), for low temperatures and large crystals the spectrum of elementary spin excitations is close to the spectrum of spin waves.<sup>23</sup> For an infinite crystal and  $T = 0$  we found  $\alpha = 1.70494$  and  $C_2 = -C_1 = 0.206734$ . In this case in Eq. (21) the parameter  $\Delta = 0$  and the excitation frequency vanishes in the two points of the Brillouin zone,  $\mathbf{k} = (0, 0)$  and  $(\pi, \pi)$  (here and below the intersite distance is taken as the unit of length). For any nonzero temperature  $\Delta$  becomes finite which generates a gap at the  $(\pi, \pi)$  point. It can be shown<sup>9,21</sup> that the gap leads to the exponential decay of spin correlations with distance and the respective correlation length is defined by the magnitude of the gap. Thus, in agreement with the Mermin-Wagner theorem<sup>16</sup> for a nonzero temperature the long-range antiferromagnetic order is destroyed in the considered two-dimensional system.

Now let us calculate the polarization operator  $\Pi(\mathbf{k}\omega)$ , Eq. (18). Using the decoupling which is equivalent to the Born approximation<sup>8</sup> and the relations

$$\langle a_{\mathbf{k}\sigma}(t)a_{\mathbf{k}\sigma}^\dagger \rangle = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} e^{\beta\omega} n_F(\omega) A(\mathbf{k}\omega), \quad \langle a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}(t) \rangle = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} n_F(\omega) A(\mathbf{k}\omega), \quad (26)$$

we find

$$\begin{aligned} \text{Im } \Pi(\mathbf{k}\omega) &= \frac{\pi}{\omega} \sum_{\mathbf{k}'} f_{\mathbf{k}'\mathbf{k}}^2 \int_{-\infty}^{\infty} d\omega' [n_F(\omega') - n_F(\omega' - \omega)] A(\mathbf{k}' - \mathbf{k}, \omega' - \omega) A(\mathbf{k}'\omega'), \\ \text{Re } \Pi(\mathbf{k}\omega) &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \Pi(\mathbf{k}\omega')}{\omega' - \omega}, \end{aligned} \quad (27)$$

where  $A(\mathbf{k}\omega) = -\pi^{-1} \text{Im } G(\mathbf{k}\omega)$  is the hole spectral function,  $n_F(\omega) = [\exp(\beta\omega) + 1]^{-1}$ ,  $f_{\mathbf{k}'\mathbf{k}} = 2tN^{-1/2}(\gamma_{\mathbf{k}'} - \gamma_{\mathbf{k}'-\mathbf{k}})(s_{\mathbf{k}}^z, s_{-\mathbf{k}}^z)^{-1/2}$  and  $\mathcal{P}$  indicates Cauchy's principal value of the integral. We notice that Eq. (27) is close in its form to the polarization operator obtained for the  $t$ - $J$  model in the spin-wave approximation.<sup>8,10</sup> We cannot directly compare the interaction constants, because the definition of the spin Green's function in this paper differs from the magnon Green's functions in Refs. 8,10. However, we notice that the spin-wave interaction constant and the respective quantity  $f_{\mathbf{k}'\mathbf{k}}^2 \omega_{\mathbf{k}}^{-1}$  in Eq. (27) are of the same order of magnitude and tend to zero linearly with  $|\mathbf{k}|$  when  $|\mathbf{k}| \rightarrow 0$ . The spin-wave constant behaves analogously near the  $(\pi, \pi)$  point, while the quantity  $f_{\mathbf{k}'\mathbf{k}}^2 \omega_{\mathbf{k}}^{-1}$  does so only in the case of an infinite crystal and zero temperature.

## V. THE HOLE GREEN'S FUNCTION

Now let us consider the hole Green's function. To use the continued fraction representation (12) for the anticommutator Green's function  $G(\mathbf{k}t)$ , Eq. (5), the average of the anticommutator of operators has to be taken as the definition of the inner product in the recursive procedure (8). From the commutation relations (4) we find for the numerator of the continued fraction  $\langle \{a_{\mathbf{k}\sigma}, a_{\mathbf{k}\sigma}^\dagger\} \rangle = \frac{1}{2}(1 + x) = \phi$  and for the time derivative

$$i\dot{a}_{1\sigma} = \sum_{\mathbf{m}} t_{\mathbf{lm}} \left[ (1 - s_1^{-\sigma} s_1^{\sigma}) s_{\mathbf{m}}^{\sigma} + s_1^{\sigma} \right] a_{\mathbf{m}, -\sigma} - \frac{1}{2} \sum_{\mathbf{m}} J_{\mathbf{lm}} (\sigma s_{\mathbf{m}}^z s_1^{\sigma} + s_{\mathbf{m}}^{\sigma}) a_{1, -\sigma} + \mu a_{1\sigma}. \quad (28)$$

With these results we get

$$E_0 = \left\langle \left\{ i\dot{a}_{\mathbf{k}\sigma}, a_{\mathbf{k}\sigma}^{\dagger} \right\} \right\rangle \left\langle \left\{ a_{\mathbf{k}\sigma}, a_{\mathbf{k}\sigma}^{\dagger} \right\} \right\rangle^{-1} = \varepsilon_{\mathbf{k}} + \mu', \quad (29)$$

$$\varepsilon_{\mathbf{k}} = (4t\phi + 6tC_1\phi^{-1} - 3JF_1\phi^{-1})\gamma_{\mathbf{k}}, \quad \mu' = \mu + (4tF_1 - 3JC_1)\phi^{-1},$$

where  $F_1 = N^{-1} \sum_{\mathbf{k}} \gamma_{\mathbf{k}} F_{\mathbf{k}}$  and  $F_{\mathbf{k}} = \sum_{\mathbf{n}} \exp[i\mathbf{k}(\mathbf{n} - \mathbf{m})] \langle a_{\mathbf{n}}^{\dagger} a_{\mathbf{m}} \rangle$ .

The estimation of  $t$  and  $J$  based on the parameters of the extended Hubbard model<sup>24</sup> gives  $J/t$  lying in the range  $0.2 - 0.3$ . For low hole concentrations we can approximate the parameter  $C_1$  by its value in an undoped lattice. For  $T = 0.02t$  in a  $4 \times 4$  lattice  $C_1 = 0.2119$ , while in a  $20 \times 20$  lattice  $C_1 = 0.2068$ . With these parameters the unrenormalized hole dispersion can be estimated as  $\varepsilon_{\mathbf{k}} \approx -0.27t\gamma_{\mathbf{k}}$  in the former case and  $-0.47t\gamma_{\mathbf{k}}$  in the latter case. Thus the first approximation of the recursive procedure describes a band which is much narrower than the two-dimensional nearest-neighbor band in the absence of correlations  $4t\gamma_{\mathbf{k}}$ . The reason for this is the antiferromagnetic alignment of spins when the hole movement is accompanied by the spin flipping. With increasing the hole concentration  $C_1 \rightarrow 0$  and the unrenormalized dispersion tends to its uncorrelated value.

The hole Green's function reads

$$G(\mathbf{k}\omega) = \frac{\phi}{\omega - \varepsilon_{\mathbf{k}} - \mu' - \Sigma(\mathbf{k}\omega)}, \quad (30)$$

$$\Sigma(\mathbf{k}\omega) = \phi^{-1} \left\langle \left\langle A_1 | A_1^{\dagger} \right\rangle \right\rangle, \quad A_1 = i\dot{a}_{\mathbf{k}\sigma} - (\varepsilon_{\mathbf{k}} + \mu') a_{\mathbf{k}\sigma},$$

where the difference between  $A_{1t}$  and  $A_1(t)$  was neglected. Due to the mentioned smallness of  $\varepsilon_{\mathbf{k}}$  for low hole concentrations and of  $J$  in comparison with  $t$ , only the term  $N^{-1/2} \sum_{\mathbf{lm}} \exp(-i\mathbf{k}\mathbf{l}) t_{\mathbf{lm}} \left[ (1 - s_1^{-\sigma} s_1^{\sigma}) s_{\mathbf{m}}^{\sigma} + s_1^{\sigma} \right] a_{\mathbf{m}, -\sigma}$  may be retained in  $A_1$  in the calculation of  $\left\langle \left\langle A_1 | A_1^{\dagger} \right\rangle \right\rangle$ . The terms in  $A_1$  which are linear in spin operators produce the following contribution to the self-energy:

$$\frac{32t^2}{N\phi} \sum_{\mathbf{k}'} \iint_{-\infty}^{\infty} d\omega_1 d\omega_2 \frac{n_F(-\omega_1) + n_B(\omega_2)}{\omega - \omega_1 - \omega_2 + i\eta} (\gamma_{\mathbf{k}} + \gamma_{\mathbf{k}-\mathbf{k}'})^2 A(\mathbf{k} - \mathbf{k}', \omega_1) B(\mathbf{k}', \omega_2).$$

Up to the prefactor this expression coincides with the respective term in the hole self-energy calculated in the spin-wave approximation.<sup>10</sup>

The term with three spin operators in  $A_1$  produces terms in the self-energy which contain two- and three-spin Green's functions. To calculate these functions one would have to solve the respective self-energy equations which could be derived in the same way as the equations in the previous section. However, such program would essentially complicate the calculation procedure. One of the possible ways to overcome this difficulty is to use the decoupling in the same manner as we applied it in the previous section, this time in the term with three spin operators in  $A_1$ . However, the comparison with the exact diagonalization data shows that this approximation does not give satisfactory results. Another way of simplification is

suggested by the above observation that the terms with the one-spin Green's function in self-energy (30) are similar to the terms obtained in the spin-wave approximation. This gives grounds to suppose that the correcting terms containing two- and three-spin Green's functions can be approximated by the respective terms of the spin-wave approximation modified for short-range antiferromagnetic order. Using the results of Refs. 10,25 and Eqs. (24), (26) we find

$$\begin{aligned}
\text{Im } \Sigma(\mathbf{k}\omega) &= \frac{16\pi t^2}{N\phi} \sum_{\mathbf{k}'} \int_{-\infty}^{\infty} d\omega' [n_B(-\omega') + n_F(\omega - \omega')] \sqrt{\frac{1 + \gamma_{\mathbf{k}'}}{\Delta + 1 - \gamma_{\mathbf{k}'}}} \\
&\times \left[ (\gamma_{\mathbf{k}-\mathbf{k}'} + \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 - \gamma_{\mathbf{k}'}}{\Delta + 1 + \gamma_{\mathbf{k}'}}} + \text{sgn}(\omega') (\gamma_{\mathbf{k}-\mathbf{k}'} - \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 + \gamma_{\mathbf{k}'}}{\Delta + 1 - \gamma_{\mathbf{k}'}}} \right]^2 \\
&\times A(\mathbf{k} - \mathbf{k}', \omega - \omega') B(\mathbf{k}'\omega'), \\
\text{Re } \Sigma(\mathbf{k}\omega) &= \mathcal{P} \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{\text{Im } \Sigma(\mathbf{k}\omega')}{\omega' - \omega}.
\end{aligned} \tag{31}$$

For low hole concentrations the spin spectral function in the above equation can be substituted by its value in the absence of holes,

$$B(\mathbf{k}\omega) = \frac{1}{2} \sqrt{\frac{|C_1|}{\alpha}} \sqrt{\frac{1 - \gamma_{\mathbf{k}}}{\Delta + 1 + \gamma_{\mathbf{k}}}} [\delta(\omega - \omega_{\mathbf{k}}) - \delta(\omega + \omega_{\mathbf{k}})]. \tag{32}$$

With this substitution and for low temperatures Eq. (31) acquires the form

$$\begin{aligned}
\text{Im } \Sigma(\mathbf{k}\omega) &= -\frac{8\pi t^2}{N\phi} \sqrt{\frac{|C_1|}{\alpha}} \sum_{\mathbf{k}'} \left\{ \left[ (\gamma_{\mathbf{k}-\mathbf{k}'} + \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 - \gamma_{\mathbf{k}'}}{\Delta + 1 + \gamma_{\mathbf{k}'}}} + (\gamma_{\mathbf{k}-\mathbf{k}'} - \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 + \gamma_{\mathbf{k}'}}{\Delta + 1 - \gamma_{\mathbf{k}'}}} \right]^2 \right. \\
&\times [1 + n_B(\omega_{\mathbf{k}'})] A(\mathbf{k} - \mathbf{k}', \omega - \omega_{\mathbf{k}'}) \\
&+ \left[ (\gamma_{\mathbf{k}-\mathbf{k}'} + \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 - \gamma_{\mathbf{k}'}}{\Delta + 1 + \gamma_{\mathbf{k}'}}} - (\gamma_{\mathbf{k}-\mathbf{k}'} - \gamma_{\mathbf{k}}) \sqrt[4]{\frac{1 + \gamma_{\mathbf{k}'}}{\Delta + 1 - \gamma_{\mathbf{k}'}}} \right]^2 \\
&\times n_B(\omega_{\mathbf{k}'}) A(\mathbf{k} - \mathbf{k}', \omega + \omega_{\mathbf{k}'}) \left. \right\}.
\end{aligned} \tag{33}$$

Excluding the numeric prefactor and some other small details this formula is similar to the respective formula of the spin-wave approximation.<sup>10</sup>

To check the validity of the approximations made we compare the hole spectral function calculated using Eqs. (30) and (33) for the case of one hole in a  $4 \times 4$  lattice with the available exact-diagonalization data obtained in this system.<sup>2</sup> The left panels in Fig. 2 demonstrate the results of the exact diagonalization, the right panels present our calculations. Both series of calculations were performed for the same set of parameters:  $J/t = 0.2$ ,  $t < 0$ ,  $T = 0$  and  $\eta = 0.1t$  ( $i\eta$  was added to the frequency  $\omega$  in the denominator of Green's function to visualize  $\delta$ -functions; in our calculations parameters  $C_1$  and  $\alpha$  were estimated for low but finite temperature  $T = 0.02t$ ). As can be seen from the figure, the spectral functions obtained in our calculations are in good agreement with the functions found in the exact diagonalization. This agreement is somewhat better than that achieved in the spin-wave approximation,<sup>7</sup> because in contrast to this approximation our approach takes into account

the difference between the spectral functions for wave vectors separated by  $(\pi, \pi)$  [cf. the spectra for  $\mathbf{k} = (0, 0)$  and  $(\pi, \pi)$ ]. As can be seen, in our approximation the binding energy of the quasiparticle peak is underestimated in comparison with the exact-diagonalization result. This may be connected with the fact that the considered hole concentration  $x = 1/16$  is not low enough and can lead to some deviations from the used spin spectral function (32).

An example of the one-hole zero-temperature spectra in a larger lattice is given in Fig. 3. We notice that the shapes of the spectra cease to change perceptibly with increasing lattice size starting from a  $16 \times 16$  lattice. Excluding the mentioned difference in spectra with wave vectors spaced by  $(\pi, \pi)$  they are close to those obtained in the spin-wave approximation.<sup>7</sup>

With the use of the Hubbard operators equations similar to Eq. (31) were obtained also in Ref. 26 for the two-dimensional  $t$ - $J$  model and in Ref. 27 for a somewhat different model of the  $\text{CuO}_2$  plane. The interaction constant derived in the former work differs from the constant in Eq. (31). The constant of Ref. 26 is not applicable for low hole concentration: the spectral functions calculated with it differ essentially from those obtained by the exact diagonalization<sup>2</sup> and in the spin-wave approximation.<sup>7,8</sup> However, this constant can be applicable in the region of heavy doping.

## VI. CONCLUDING REMARKS

Equation (31) was obtained under the supposition of a small hole concentration. We have verified that in this limit Eq. (31) in combination with Eq. (30) describes the hole spectral function in good agreement with the exact diagonalization data. On the other hand, with increasing hole concentration spin correlations are weakened, the self-energy becomes small and elementary excitations described by the two equations tend to the weakly correlated nearest-neighbor band with the dispersion  $\varepsilon_{\mathbf{k}}$ , Eq. (29), where  $C_1 \rightarrow 0$ . Thus, the obtained equations give the correct behavior of the hole spectrum in the two limiting cases. Besides, it was demonstrated that Eqs. (17) and (21) with the parameters determined self-consistently give a quantitatively correct description of the spin subsystem in the undoped case. Equations of the spin-wave approximation, which are similar to Eqs. (17), (21) and (27), describe the rapid weakening of spin correlations with hole doping,<sup>10</sup> as it is necessary for the above-discussed transformation of the hole spectrum from light to heavy doping. This gives ground to suppose that the obtained equations can provide a qualitatively correct interpolation between these two limiting cases.

## ACKNOWLEDGMENTS

This work was partially supported by the ESF grant No. 4022 and by the WTZ grant (Project EST-003-98) of the BMBF. A.S. thanks International University Bremen for hospitality.

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## FIGURES

FIG. 1. The spin correlations  $\mathcal{C}(l) = 4|\langle s_{\mathbf{l}}^z s_{\mathbf{0}}^z \rangle|$ ,  $\mathbf{l} = (l, 0)$  calculated for  $T/J = 0.5, 0.75$  and 1 in this work (open circles) and by the Monte Carlo method in Ref. 14 (filled circles). In both calculations a  $32 \times 32$  lattice without holes was used.

FIG. 2. The hole spectral function  $A(\mathbf{k}\omega)$  for the case of one hole in a  $4 \times 4$  lattice and parameters  $J = 0.2t$ ,  $\eta = 0.1t$ , and  $T = 0$ . Left panels: exact-diagonalization data from Ref. 2, right panels: our calculations. The respective wave vectors are indicated in the upper right corners of the panels.

FIG. 3. The hole spectral function  $A(\mathbf{k}\omega)$  for the case of one hole in a  $20 \times 20$  lattice and parameters  $J = 0.2t$ ,  $\eta = 0.01t$ , and  $T = 0$ . Wave vectors indicated near the curves are selected along the symmetry lines  $(0, 0) - (0, \pi)$  in (a) and  $(0, 0) - (\pi, \pi)$  in (b).









